Russian Journal of General Chemistry 2007 vol.77 N12, pages 2130-2139

Fourier transform IR spectra and structure of 2-substituted 1-nitro- and 1-bromo-1-nitroethenes

Gazizova A., Shagidullin R., Chernova A., Vereshchagina Y., Chachkov D., Ishmaeva E., Berestovitskaya V.

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

Molecular structure and vibrational spectra of 2- trichloromethyl(ethoxycarbonyl)-1-nitroethenes and 2- trichloromethyl(ethoxycarbonyl)-1-bromo-1-nitroethenes were calculated in terms of the density functional theory (B3LYP/6-31G*). The experimental FTIR spectra of these compounds in the range from 4000 to 400 cm-1 were interpreted in detail on the basis of the calculation data. 2-Substituted 1-nitro- and 1-bromo-1-nitroethenes were assigned the structure with trans orientation of the nitro and trichloromethyl (or ethoxycarbonyl) groups, and the ethoxycarbonyl derivatives were assumed to exist in equilibrium between s-cis and s-trans conformers. © 2007 Pleiades Publishing, Ltd.

http://dx.doi.org/10.1134/S1070363207120109